

Article

Evaluation of the Inhibitory Efficiency of Yohimbine on Corrosion of OLC52 Carbon Steel and Aluminum in Acidic Acetic/Acetate Media

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Abstract

The present study assesses the effectiveness of the indole-type alkaloid Yohimbine (YHB) as a green corrosion inhibitor for OLC52 carbon steel and Al in 0.25/0.25 mol L^{−1} acetic acid/potassium acetate solutions relevant for de-icing applications. Electrochemical techniques, including cyclic and linear sweep voltammetry, chronoamperometry, and electrochemical impedance spectroscopy have been combined with the evaluation of adsorption isotherms and molecular modeling calculations. YHB significantly decreases the corrosion rate for both metals, attaining inhibitory efficiencies of up to 95% for OLC52 and 91% for Al at 298 K, while maintaining high protection efficiency even at higher temperatures. The Langmuir adsorption model and the values of ΔG_{ads}^0 between -31 and -41 kJ mol^{−1} indicate a spontaneous adsorption process defined by a mixed physicochemical mechanism, resulting in the formation of a compact protective film. Quantum molecular descriptors support the ability of YHB molecules to interact with metal surfaces via donor–acceptor interactions and electrostatic interactions. The findings demonstrate the potential of YHB as an environmentally friendly inhibitor for the protection of ferrous and non-ferrous alloys in mildly acidic acetic/acetate media used in de-icing solutions.

Keywords: corrosion inhibitor; electrochemical methods; yohimbine; quantum chemical calculations; Langmuir adsorption isotherm



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1. Introduction

Metal corrosion is an unavoidable phenomenon that negatively impacts the economy and technological systems, impacting infrastructure elements in sectors such as construction, aerospace, and petrochemicals, resulting in losses of 3%–4% of worldwide GDP [1,2]. Corrosion prevention is a critical concern, with the best-known methods being cathodic protection and metal coatings; nonetheless, the related costs are considerable and not universally applicable to all metal designs. In contrast, organic inhibitors represent a more cost-effective approach to anti-corrosion protection, as they reduce direct corrosive attacks on the metal through the adsorption of the organic component at the metal/aggressive solution interface, thereby forming a protective film [3,4].

Research interest in green corrosion inhibitors has notably increased owing to their biodegradability, low environmental toxicity, and plant-derived origins [5]. Natural extracts consist of organic compounds that exhibit corrosion-inhibiting effects, including

flavonoids, terpenoids, polyphenols, and alkaloids [6,7]. They exhibit a structure containing heteroatoms such as nitrogen, sulfur, or oxygen, or contain conjugated double bond systems. Due to their presence, adsorption occurs at the metal surface, hence reducing the anodic or cathodic processes at that surface [8]. A considerable proportion of natural substances or plant extracts cited in the literature, utilized in harsh acidic or saline solutions, demonstrate *IE* values exceeding 80%–90% [9].

Alkaloids are organic compounds characterized by the presence of nitrogen atoms in their structure, which have physiological effects on animal beings. Their heterocyclic structure, characterized by aromatic properties and the presence of nitrogen, enhances interaction with metallic substrates. The literature indicates that natural extracts containing alkaloids have been successfully identified as efficient corrosion inhibitors for steel in acidic environments, achieving *IE* of over 90% [10,11]. Synthetically derived compounds with a similar indolic structure have demonstrated effectiveness as inhibitors in acidic environments of HCl and H₂SO₄ [12].

Yohimbine (YHB), a natural alkaloid characterized by an indolic structure, is a primary constituent of the bark of the *Pausinystalia johimbe* tree and is also found in certain species of *Rauwolfia* [13]. Structurally, the presence of the indole nucleus, hydroxyl groups, and nitrogen atoms indicates the potential for adsorption on metal surfaces, implying a mixed adsorption mechanism [8]. As of now, no scientific articles have evaluated the efficacy of YHB as a corrosion inhibitor.

The significance of the acetic/acetate medium is practically substantial, since acetates and formates are widely utilized as anti-icing and de-icing agents in airport infrastructure and aircraft, providing a less corrosive alternative to chlorinated salts [14]. Commercial treatments, including potassium acetate-based solutions (e.g., Provifrost® KA ECO - Provion Industries N.V., Hemiksen, Belgium), incorporate corrosion inhibitors to protect the treated metal structures [15]. Exposure of aluminum to CH₃COOK inhibitor solutions has shown substantial reductions in corrosion current values. Furthermore, research on metal coatings utilized in aeronautics indicates that the underlying metal structures can be protected when inhibitors are efficiently included into defroster formulations [16,17]. In parallel with the experimental studies, numerical approaches have also been developed for the analysis of corrosion and erosion–corrosion phenomena, particularly in systems with high-speed water jets and complex geometries. For example, Gok et al. reviewed the use of CFD modeling and finite element analysis (FEA) to describe erosion-induced corrosion formation in water jets [18].

Examining the corrosion inhibition mechanism of natural compounds like YHB in acetic/acetate media is fundamentally significant for advancing research on alkaloids as potential green corrosion inhibitors and practically important for identifying applications in the protection of metal structures within the aeronautical industry.

The integration of voltammetric and electrochemical impedance spectroscopy investigations with molecular modeling is essential for elucidating adsorption mechanisms and providing a first evaluation of the capacity of the examined compounds to prevent metal corrosion [19]. Techniques such as DFT provide relevant molecular descriptors, including the energy of the highest occupied molecular orbital (*E*_{HOMO}), the energy of the lowest unoccupied molecular orbital (*E*_{LUMO}), electronegativity, hardness, and softness, which clarify the relationship between the structure and inhibitory properties of the studied organic compound [20].

This study aims to assess the inhibitory efficacy of YHB on the corrosion of OLC52 carbon steel and aluminum in 0.25/0.25 mol L^{−1} acetic acid/potassium acetate solutions, utilizing electrochemical techniques such as cyclic voltammetry, linear voltammetry, chronoamperometry, and electrochemical impedance spectroscopy, in conjunction with theoretical

molecular modeling calculations. The findings would enable the integration of natural alkaloids as environmentally sustainable corrosion inhibitors and their application in the protection of metallic components across many sectors.

2. Materials and Methods

2.1. Materials

YHB has $C_{21}H_{26}N_2O_3$ as its chemical formula and is named according to IUPAC methyl(1S,15R,18S,19R,20S)-18-hydroxy-1,3,11,12,14,15,16,17,18,19,20,21-dodecahydroyohimban-19-carboxylate hydrochloride. YHB is an indole alkaloid derived from the root of the *Pausinystalia johimbe* tree [21]. It is commercially available as standard yohimbine hydrochloride with a concentration of $\geq 98\%$ HPLC, produced by Sigma-Aldrich® (St. Louis, MO, USA). Figure 1 illustrates the chemical structure of YHB.

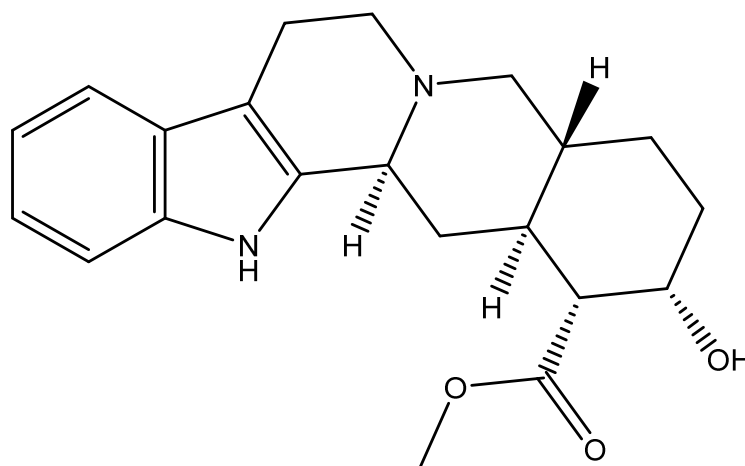


Figure 1. Chemical structure of YHB.

Yohimbine hydrochloride exhibits significant stability in neutral or mildly acidic aqueous environments (pH = 5–6), while in strongly acidic conditions it undergoes hydrolytic degradation. Light influences degradation through photooxidation resulting in the formation of 3,14-dehydroyohimbin. The stability is enhanced by storage in airtight ferrite containers [22].

Electrochemical measurements were conducted using a BioLogic SP150 potentiostat (BioLogic Science Instruments, Seyssinet-Pariset, France) connected to a thermostatic electrochemical cell, which used a three-electrode assembly. This assembly consisted of a working electrode made from the corroded material (OLC52 and Al $p = 99\%$) with active surface areas of 0.65 cm^2 and 0.785 cm^2 , respectively, alongside two graphite counter electrodes and a Ag/AgCl reference electrode. The chemical composition of the utilized steel is presented in Table 1.

Table 1. Chemical composition of OLC52 steel.

Fe (%)	C (%)	P (%)	S (%)	Mn (%)	Si (%)
97.60	0.20	0.050	0.050	1.60	0.050

The corrosive environment (BS) solution utilized in the experiments comprised a solution of 0.25 mol L^{-1} acetic acid and 0.25 mol L^{-1} potassium acetate. To assess the influence of the YHB concentration on the corrosion process of the studied metals, various concentrations of inhibitor were added into the BS solution, namely 10^{-6} , 10^{-5} , 10^{-4} , $2.5 \cdot 10^{-4}$, $5 \cdot 10^{-4} \text{ mol L}^{-1}$ YHB; the pH of the test solutions maintained at 4.75, con-

sistent with that of the corrosive media employed. The reactants used were acetic acid (glacial), 100%, Suprapure® (Merck, Rahway, NJ, USA), potassium acetate, ACS reagent, $\geq 99.0\%$ (Sigma-Aldrich) and the corrosion inhibitor was YHB, in the form of yohimbine hydrochloride $\geq 98\%$ (HPLC), powder, produced by Merck. The solutions were prepared by dissolving in BS a quantity of YHB corresponding to a concentration of $10^{-2} \text{ mol L}^{-1}$ (stock solution), followed by successive dilutions, in order to prepare the test solutions.

2.2. Electrochemical Methods

The electrochemical measurements were conducted utilizing the BioLogic SP-150 potentiostat, which features EC-Lab v.10.23 software. Platinum electrodes were employed for cyclic voltammetry studies, as well as electrodes made from corroded materials (OLC52 and Al). The Pt electrode was polarized at scan rates of 100, 50, and 10 mV s^{-1} , whilst the OLC52 and Al were polarized at 100 mV s^{-1} . The utilized potential ranges were -1 to 2.25 V for Pt and OLC52, and -1 to 1.5 V for Al.

Electrochemical investigations, including linear sweep voltammetry, chronoamperometry, chronopotentiometry, and electrochemical impedance spectroscopy, are utilized to determine characteristics such as corrosion currents, corrosion rates, and inhibition efficiency (IE). The data obtained were then utilized for the graphical representations of the isotherms and the Arrhenius diagrams. The electrochemical measurements were conducted at controlled temperatures, utilizing a Julabo F5 thermostat bath, which maintains a temperature stability of $\pm 0.1 \text{ K}$. Prior to each electrochemical measurement, the working electrode underwent sequential grinding treatments using Si-C sanding paper of grits of 120, 240, 600, 1200, 2400, and 4000. Thereafter, the working electrode was subjected to ultrasonication, alcohol washing, and drying. Prior to each measurement, the cell containing 100 mL of test solution was deaerated by purging N_2 for 10 min to minimize the amount of dissolved oxygen. Prior to initiating linear voltammetry measurements, the working electrode underwent a chronopotentiometry technique for 3600 s to stabilize the potential. Each experimental measurement was plotted three times to ensure reproducibility, and the standard deviation of the three determinations is reported for each parameter.

The linear sweep voltammograms obtained at a corrosion rate of 1 mV s^{-1} , in the potential range of -250 mV to $+250 \text{ mV}$ versus E_{OCP} , were logarithmically converted to obtain the cathodic and anodic Tafel slopes, which were then used to determine the corrosion current density and the corrosion rate. The convergence of these slopes yields data on the i_{corr} corrosion current and the E_{corr} corrosion potential, with these results derived from the corrosion module integrated within the EC-Lab potentiostat program.

The IE was calculated from the corrosion currents utilizing Equation (1), both in the presence and absence of YHB [23].

$$IE = \frac{i_{\text{corr}} - i_{\text{corr}(\text{inhib})}}{i_{\text{corr}}} \times 100\% \quad (1)$$

where

IE —inhibitory efficacy of YHB [%];

i_{corr} , $i_{\text{corr}(\text{inhib})}$ —the corrosion current in the case of the uninhibited process, respectively, in the presence of the YHB inhibitor [A m^{-2}].

The corrosion mechanism at the OLC52 interfaces, specifically in the Al/acetic acetate solution, was examined using electrochemical impedance spectroscopy (EIS) performed at open circuit potential (E_{OCP}) values, across frequencies ranging from 100 kHz to 10 mHz , with an alternating current oscillation amplitude of 10 mV rms . The spectra were plotted at 60 points, logarithmically distributed with 10 points each decade, to be fitted into an equivalent electrical circuit using a complex nonlinear least squares method, namely

the Levenberg–Marquardt algorithm using ZView 4.0 software (Scribner Associates, Inc., Southern Pines, NC, USA) [24,25].

2.3. Molecular Modeling

The voltametric experiments were completed using theoretical molecular modeling calculations conducted with Hyperchem 8.0 software (Hypercube Inc., Boulder, CO, USA, Scientific Software). The YHB molecule was modeled in both a vacuum and aqueous environment utilizing Density Functional Theory with the B3LYP functional and a 6-31G* basis set. This method facilitated the plotting of the frontier orbitals, specifically the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and the computation of molecular descriptors, including E_{HOMO} , E_{LUMO} , the HOMO–LUMO energy gap (ΔE), absolute electronegativity (χ), chemical hardness (η), chemical softness (σ), and dipole moment (μ) for the YHB molecule [26].

The ionization energy and electron affinity were obtained from the energy levels of the Frontier orbitals using Equations (2) and (3), respectively. [27].

$$I = -E_{\text{HOMO}} \quad (2)$$

$$A = -E_{\text{LUMO}} \quad (3)$$

The interaction of YHB with a prospective metallic surface has been clarified using the descriptors “ χ , η , and σ .” Chemical hardness (“ η ”) assesses the resistance of YHB molecules to charge transfer, reflecting their durability, whereas chemical softness (“ σ ”) provides insights on electron exchange with the metal surface [28]. These are obtained via ionization energy and electron affinity as per Equations (4)–(6).

$$\chi = \frac{I + A}{2} \quad (4)$$

$$\eta = \frac{I - A}{2} \quad (5)$$

$$\sigma = \frac{1}{\eta} \quad (6)$$

The mechanism by which the YHB molecule may inhibit further attacks from the corrosive media on the metal surface is illustrated by the molecular surface and molecular volume. The former is obtained using the QSAR properties module of Hyperchem software. Acquiring structure–property connections offers both a supplement to voltammetric experiments and a means to evaluate the inhibition mechanism [29].

3. Results

3.1. Cyclic Voltammetry

To investigate the electrochemical behavior of YHB, particularly its stability, in the potential domain between the oxygen release process and hydrogen, cyclic voltamograms were plotted on the electrodes of Pt, carbon steel OLC52 and Al, in the BS, respectively, in the presence of inhibitor concentrations 10^{-6} , 10^{-5} , 10^{-4} , $5 \cdot 10^{-4}$ mol L^{−1}. Figure 2a–c show the cyclic voltamograms plotted on the Pt electrode, at the scanning rates of 100, 50, and 10 mV s^{−1}, respectively.

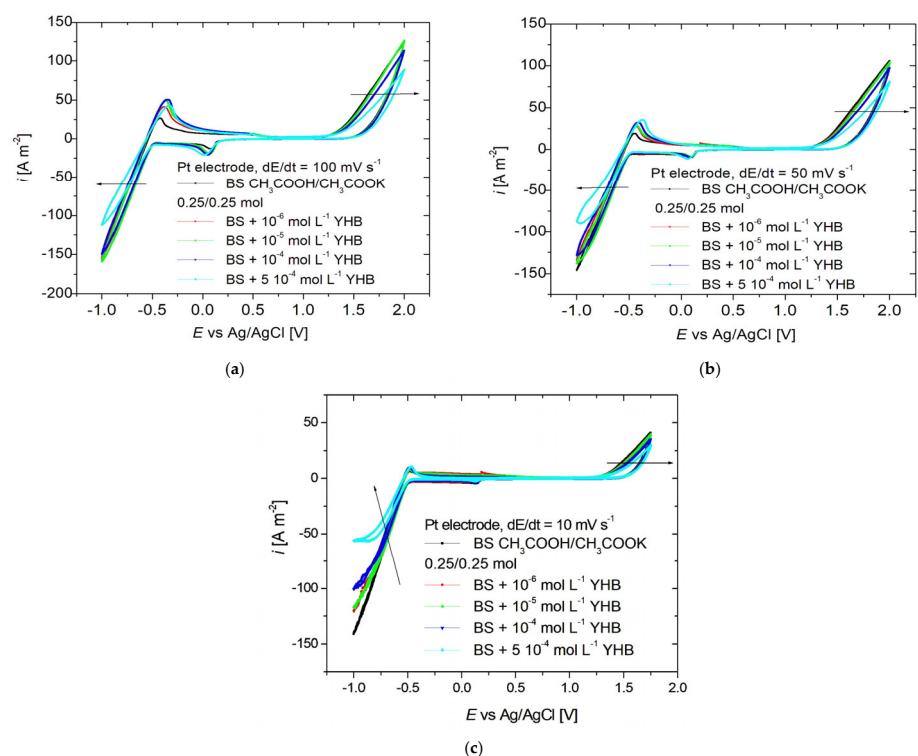


Figure 2. Cyclic voltammograms on Pt electrode in the presence and absence of various concentrations of YHB at the scan rates (a) 100 mV s^{-1} , (b) 50 mV s^{-1} , (c) 10 mV s^{-1} .

They have the specific shape of voltammograms in acetic acetate medium. In the absence of YHB, starting with potential values above $+1.4 \text{ V vs. Ag/AgCl}$, on the anode branch there is a peak associated with oxygen release, followed in the reverse branch by the peak corresponding to the reduction in Pt oxides formed on the surface (around 0 V vs. Ag/AgCl), ultimately culminating in the hydrogen evolution process.

Increasing YHB concentration gradually decreases both anode and cathode current densities, indicating YHB adsorption at the electrode interface and reduced charge transfer. The scanning rate significantly affects the allure and intensity of the curves; particularly, at 100 mV s^{-1} , distinct peaks are observed, whereas at 10 mV s^{-1} , the curves become flattened, indicating a quasi-equilibrium condition and the predominance of diffusional control. To highlight the inhibition of both branches, cyclic voltammograms are presented separately for the anodic (Figure 3a) and cathodic (Figure 3b) domains. In the presence of YHB, the currents in both regions decrease, consistent with the formation of a stable adsorbed organic film.

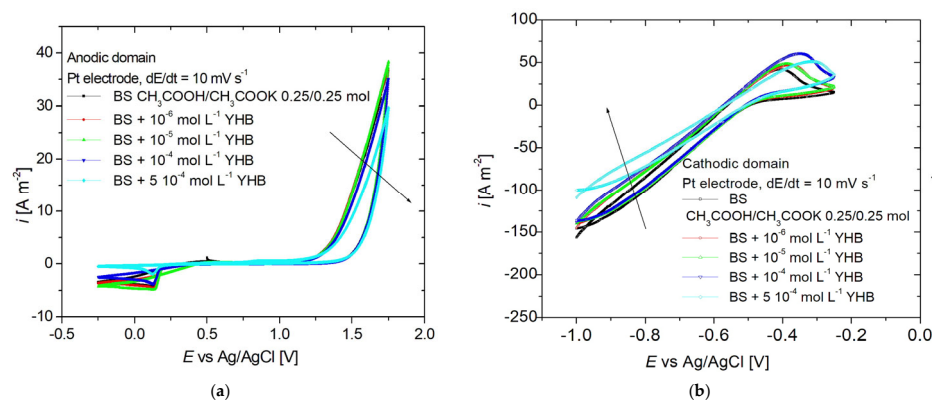


Figure 3. Anodic (a) and cathodic (b) domains plotted at 10 mV s^{-1} .

The voltammograms obtained from the OLC52 carbon steel at a scan rate of 100 mV s^{-1} , as illustrated in Figure 4a–c, demonstrate greater currents compared to those observed with platinum, signifying the dissolution process of iron $\text{Fe} \rightarrow \text{Fe}^{2+}$ and the subsequent formation of iron oxides. Compared to Pt, cyclic voltammograms for OLC52 show much higher current values associated with iron dissolution and oxide formation. The presence of YHB significantly reduces them, indicating the effective obstruction of active dissolution sites on the steel surface.

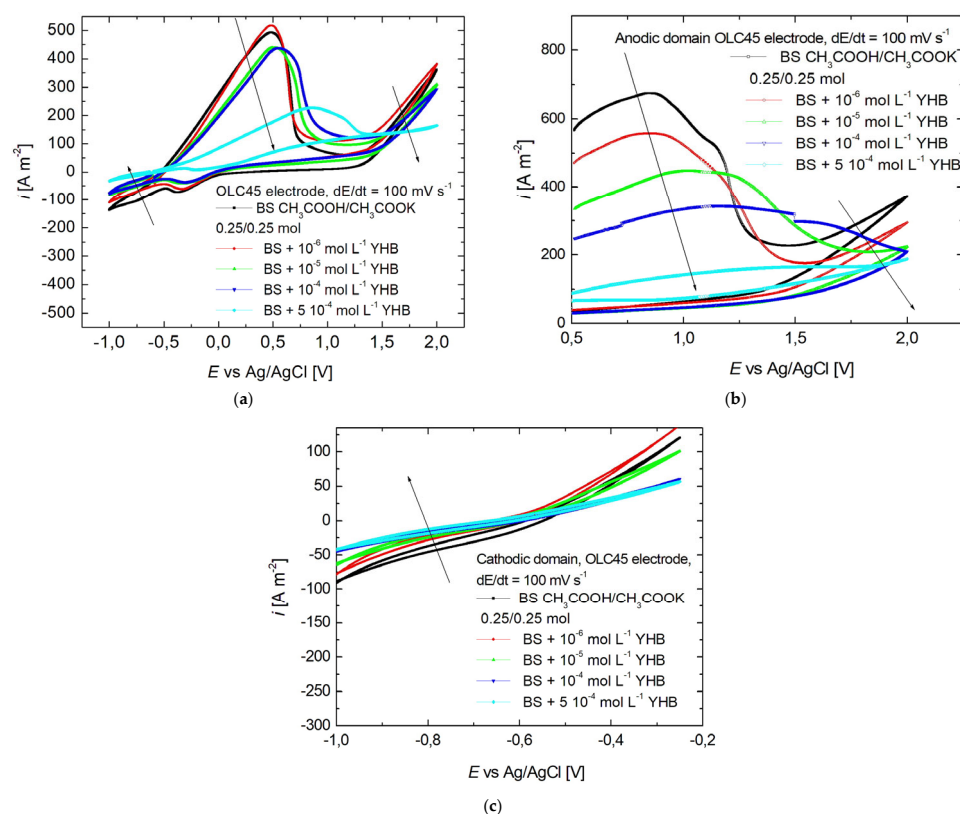


Figure 4. Cyclic voltammograms on OLC52 electrode in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 mol L^{-1} solution in the absence and presence of YHB at concentrations 10^{-6} M , 10^{-5} M , 10^{-4} M , $5 \cdot 10^{-4} \text{ M}$, polarization rate 100 mV s^{-1} : (a) whole representation, (b) anodic domain, (c) cathodic domain.

In the anodic branch, as illustrated in Figure 4b, it is observed that the droplets become indistinct and the oxygen release potentials shift towards more positive values with increasing inhibitor concentration, indicating the inhibition of metal dissolution due to the adsorption of the inhibitor.

In the cathodic branch (Figure 4c), the shift in the specific potential of hydrogen evolution indicates that YHB acts as a mixed inhibitor, attributable to the heteroatoms (O, N) in its structure, the presence of the benzene ring, and the ether groups, which reduce the electrochemical activity of the steel [30]. The voltammograms obtained from the aluminum electrode are illustrated in Figure 5a–c, at a polarization rate of 100 mV s^{-1} , displaying characteristics typical of passivable metals. During anodic polarization in an acidic environment, the increase in the current density value is due to the active dissolution and the destruction of its native oxide layer and not to the formation of a stable Al_2O_3 layer. Aluminum does not passivate in acidic conditions, where pitting corrosion occurs immediately after anodic polarization [31].

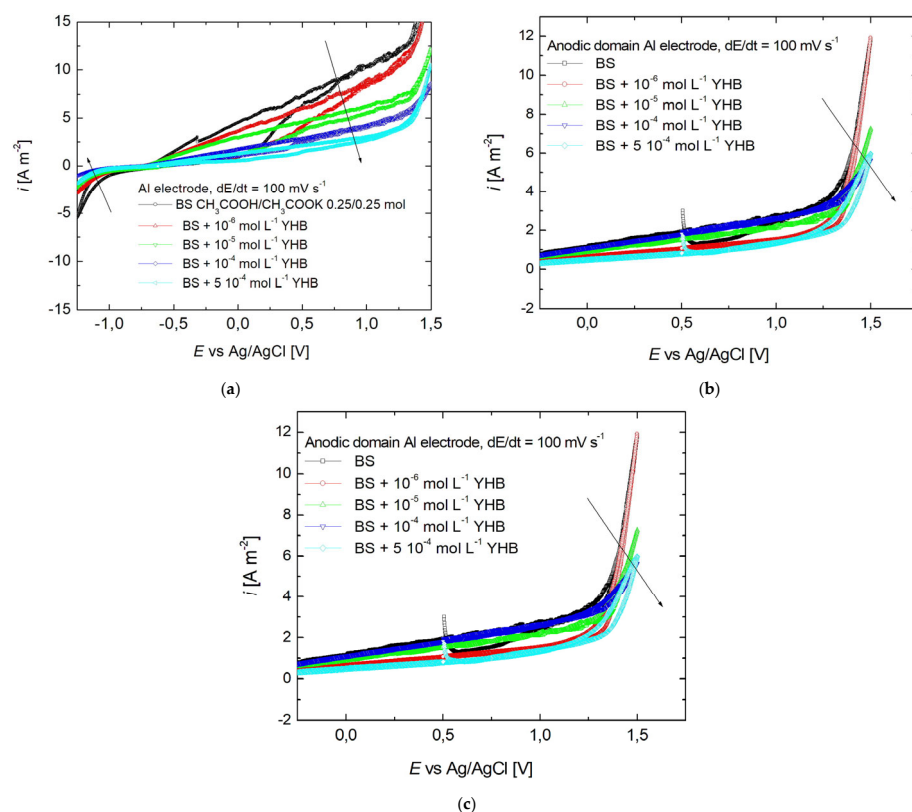


Figure 5. Cyclic voltammograms on Al electrode in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 mol L^{-1} solution in the absence and presence of YHB at concentrations 10^{-6} M, 10^{-5} M, 10^{-4} M, $5 \cdot 10^{-4}$ M, polarization rate 100 mV s^{-1} : (a) whole representation, (b) anodic domain, (c) cathodic domain.

During the cathodic scan, the reduction in H^+ and the release of hydrogen are observed. In the presence of YHB, the anode and cathode characteristics shift, and the current–potential diagrams become smoother, reflecting the adsorption of YHB, the consolidation of the oxide layer and the change in electrode kinetics. The YHB molecule adsorbs onto the aluminum oxide layer, enhancing the passive film, which consequently reduces the current density. At high inhibitor concentrations, an effective surface coating is apparent, yielding an organic film that impedes the incursion of corrosive ions (acetate and protons) towards the metallic substrate.

In all cases, the evolution of the electrochemical response towards a lower reactivity with the increase in the concentration of YHB is consistent with its molecular structure, which contains conjugated rings and heteroatoms of nitrogen and oxygen. This facilitates the adsorption of the organic substance onto metal surfaces via potential donor–acceptor interactions and hydrogen bonding [32]. The cyclic voltammograms indicate that YHB exhibits mixed inhibitory activity, influencing both anodic and cathodic processes, and remains stable within the working potential range. This phenomenon is specific to inhibitors that act by blocking the active sites at the metal–solution interface, rather than by a shift from a purely anodic to a purely cathodic control.

3.2. Linear Sweep Voltammetry

The Tafel diagrams were acquired following nitrogen bubbling for 10 min to eliminate dissolved oxygen ions and avert side reactions, followed by potential stabilization by chronopotentiometry until a stationary state was reached. Figure 6a illustrates the Tafel diagrams for the $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 mol L^{-1} solution, both in the absence and presence of varying concentrations of YHB, at a polarization rate of 1 mV s^{-1} .

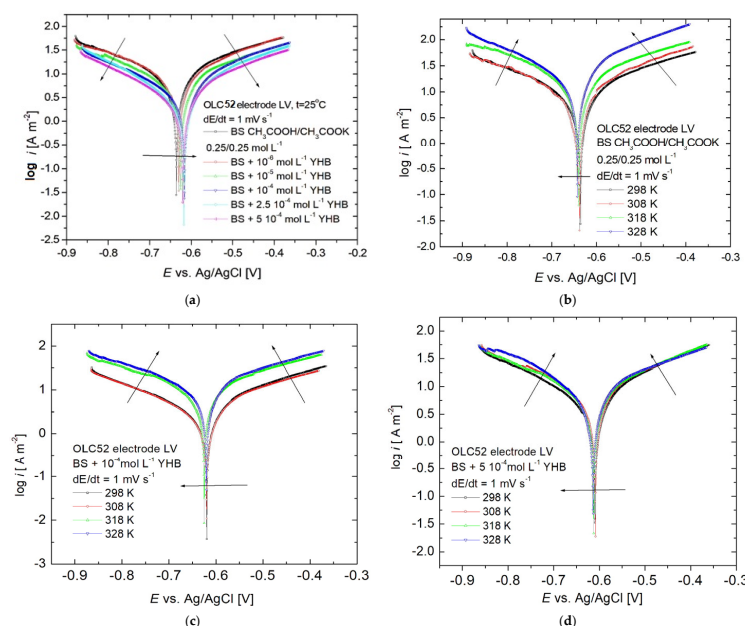


Figure 6. Tafel diagrams on the OLC52 electrode in test solutions at polarization rate of 1 mV s⁻¹: (a) concentration influence, (b) temperature influence for BS, (c) BS + 10⁻⁴ mol L⁻¹, (d) BS + 5 · 10⁻⁴ mol L⁻¹.

The BS solution reveals higher corrosion currents and a notable current density at both anodic and cathodic potentials, indicating an active process of iron dissolution and hydrogen evolution. The addition of YHB results in a shift in the Tafel curves towards reduced current densities, with significant decreases in the cathodic slope (b_c) and anodic slope (b_a), suggesting the concurrent inhibition of both anodic and cathodic processes, thereby characterizing YHB as a mixed inhibitor.

The electrochemical measurements in Table 2 indicate a progressive reduction in the i_{corr} corrosion current from 764.4 $\mu\text{A cm}^{-2}$ to 38.2 $\mu\text{A cm}^{-2}$ at a concentration of 5 · 10⁻⁴, yielding an IE of 95%. The reduced shifts in corrosion potential, correlated with the simultaneous reduction in anode and cathodic currents substantiate the classification of YHB as a mixed-type inhibitor, which is in agreement with the results of cyclic voltammetry and EIS.

Table 2. Tafel parameters characteristic of OLC52 carbon steel corrosion process in test solutions.

Metal	T [K]	YHB conc.	i_{corr}	E_{corr}	$-b_c$	b_a	v_{corr}	IE	θ
			[$\mu\text{A cm}^{-2}$]	[mV]	[mV dec ⁻¹]	[mV dec ⁻¹]	[mm y ⁻¹]		
OLC52	298	BS	764.4 ± 15.27	-635.6 ± 2.01	286.3 ± 5.31	236.2 ± 3.0	8.89 ± 0.180	-	-
		10 ⁻⁶ M	637. ± 7.91	-633.0 ± 1.14	237.8 ± 9.8	223.4 ± 8.5	7.41 ± 0.092	16.6	0.17
		10 ⁻⁵ M	576.6 ± 1.69	-625.1 ± 2.56	200.1 ± 6.6	150.3 ± 4.9	6.71 ± 0.021	24.6	0.25
		10 ⁻⁴ M	256.9 ± 2.90	-619.4 ± 2.08	194.1 ± 4.1	148.2 ± 3.0	2.99 ± 0.339	66.4	0.66
		2.5 · 10 ⁻⁴ M	198.8 ± 19.4	-621.4 ± 1.29	171.9 ± 10.3	125.8 ± 4.4	2.31 ± 0.226	74.0	0.74
		5 · 10 ⁻⁴ M	38.2 ± 3.18	-618.4 ± 3.18	15.4 ± 1.7	12.1 ± 2.2	0.44 ± 0.039	95.0	0.95
	308	BS	837.6 ± 33.71	-640.1 ± 0.96	295.4 ± 14.3	239.3 ± 0.6	9.74 ± 0.388	-	-
		10 ⁻⁶ M	644.3 ± 34.69	-633.8 ± 1.98	270.3 ± 13.8	237.5 ± 2.6	7.49 ± 0.391	23.1	0.23
		10 ⁻⁵ M	617.6 ± 25.68	-625.5 ± 2.94	203.8 ± 2.8	154.9 ± 2.3	7.18 ± 0.297	26.3	0.26
		10 ⁻⁴ M	265.7 ± 8.80	-618.9 ± 0.34	203.3 ± 19.7	145.5 ± 2.6	2.49 ± 0.246	68.3	0.68
		2.5 · 10 ⁻⁴ M	193.0 ± 16.45	-621.7 ± 1.67	198.9 ± 6.4	140.7 ± 5.6	2.24 ± 0.193	77.0	0.77
		5 · 10 ⁻⁴ M	45.9 ± 0.96	-609.2 ± 2.54	24.6 ± 0.7	17.7 ± 1.4	0.53 ± 0.011	94.5	0.95
	318	BS	1307.8 ± 12.16	-637.1 ± 1.08	273.9 ± 1.6	230.7 ± 4.3	15.20 ± 0.146	-	-
		10 ⁻⁶ M	781.4 ± 4.97	-631.8 ± 0.73	251.3 ± 7.3	298.7 ± 4.0	9.08 ± 0.053	40.2	0.40
		10 ⁻⁵ M	651.9 ± 35.30	-632.5 ± 1.66	277.5 ± 0.9	228.3 ± 0.5	7.58 ± 0.326	50.2	0.50
		10 ⁻⁴ M	273.5 ± 8.27	-621.6 ± 2.21	256.1 ± 2.9	191.9 ± 3.7	3.18 ± 0.096	79.1	0.79
		2.5 · 10 ⁻⁴ M	240.8 ± 8.40	-619.9 ± 1.96	210.1 ± 1.5	140.9 ± 5.9	2.80 ± 0.100	81.6	0.82
		5 · 10 ⁻⁴ M	65.9 ± 4.99	-612.9 ± 0.12	25.5 ± 1.2	25.7 ± 1.0	0.77 ± 0.056	95.0	0.95
	328	BS	1349.8 ± 8.04	-636.8 ± 1.73	276.5 ± 10.3	254.4 ± 14.6	15.70 ± 0.050	-	-
		10 ⁻⁶ M	1172.3 ± 27.24	-637.6 ± 1.53	225.6 ± 3.3	196.8 ± 6.0	13.63 ± 0.316	13.2	0.13
		10 ⁻⁵ M	792.5 ± 14.93	-628.9 ± 1.72	213.6 ± 2.3	180.6 ± 3.0	9.22 ± 0.174	41.3	0.41
		10 ⁻⁴ M	460.3 ± 22.17	-625.8 ± 1.10	158 ± 6.1	133.9 ± 4.5	5.35 ± 0.259	65.9	0.66
		2.5 · 10 ⁻⁴ M	241.9 ± 2.92	-618.7 ± 2.28	188.7 ± 4.3	127.4 ± 1.5	2.81 ± 0.034	82.1	0.82
		5 · 10 ⁻⁴ M	67.7 ± 10.13	-614.3 ± 1.73	27.6 ± 4.3	23.9 ± 2.0	0.79 ± 0.117	95.0	0.95

The shift in the E_{corr} corrosion potential towards more positive values indicates a minor predominance of anodic inhibition without a substantial modification in the overall process. The reduction in Tafel slopes and the corrosion rate v_{corr} indicates the establishment of a stable adsorbed coating on the surface of OLC52 steel, which limits charge transfer processes. Figure 6b depicts the effect of temperatures ranging from 298 to 328 K on the BS solution. Figure 6c,d, representing solutions with concentrations of 10^{-4} and $5 \cdot 10^{-4} \text{ mol L}^{-1}$, exhibit a much reduced rise in temperature currents, therefore confirming the inhibitor's continued efficacy at higher temperatures. Table 2 illustrates that at 328 K, i_{corr} decreases from $1349 \mu\text{A cm}^{-2}$ (BS) to $67.7 \mu\text{A cm}^{-2}$ ($5 \cdot 10^{-4} \text{ mol L}^{-1}$), while maintaining an IE of 95%, indicating the resilience of the YHB protective layer with regard to temperature.

Figure 7a illustrates the Tafel curves obtained for the Al electrode in a $0.25/0.25 \text{ mol L}^{-1}$ acetic/acetate solution at 298 K, with varying concentrations of YHB. The corrosion current in BS is $32.9 \mu\text{A cm}^{-2}$, with an E_{corr} of -556 mV versus Ag/AgCl, indicating the active dissolving of aluminum and localized perforation of the oxide layer. The addition of YHB, as illustrated in Table 3, reveals a gradual decrease in i_{corr} and a change in the E_{corr} potential towards more positive values, indicative of the predominant inhibition of the anodic process. At the final concentration of $5 \cdot 10^{-4} \text{ M}$, i_{corr} decreases to $2.8 \mu\text{A cm}^{-2}$, yielding an IE of 91.5%. The corrosion rate, v_{corr} , is markedly decreased from 0.358 mm y^{-1} to 0.03 mm y^{-1} . The Tafel curves illustrated in Figure 7b–d demonstrate that although the corrosion current density (i_{corr}) shows a marginal rise with temperature, the IE remains higher (83%–91%) at 328 K. This observation corroborates the adsorptive nature of the YHB molecules, which adhere to the aluminum oxide surface, thereby obstructing the subsequent attack of acetate ions on the passive layer. YHB effectively inhibits corrosion in the acetic/acetate environment of OLC52 and Al steel, significantly diminishing Tafel currents and demonstrating excellent efficiency at higher working temperatures, therefore confirming the formation of a thermally and electrochemically resistant protective coating.

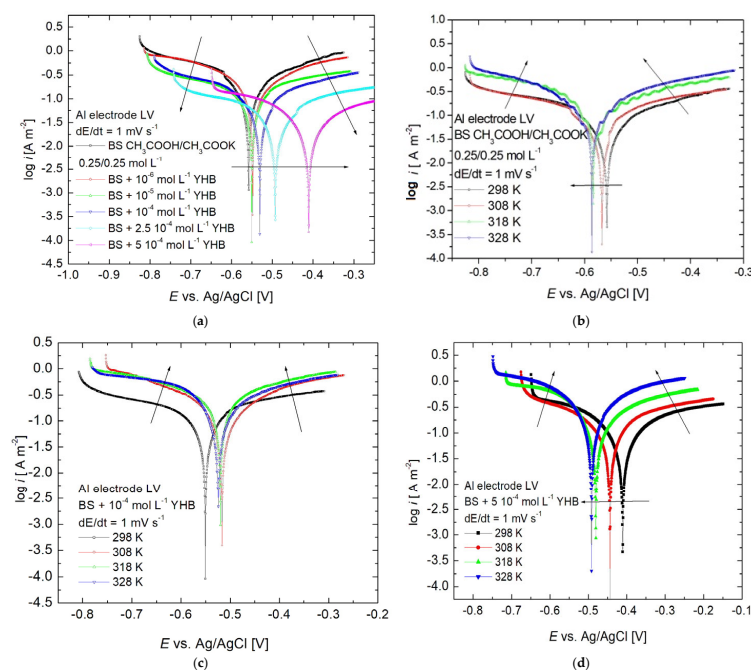


Figure 7. Tafel diagrams on the Al electrode in test solutions at polarization rate of 1 mV s^{-1} : (a) concentration influence, (b) temperature influence for BS, (c) BS + $10^{-4} \text{ mol L}^{-1}$, (d) BS + $5 \cdot 10^{-4} \text{ mol L}^{-1}$.

Table 3. Tafel parameters characteristic of Al carbon steel corrosion process in test solutions.

Metal	T [K]	YHB conc.	i_{corr}	E_{corr}	$-b_c$	b_a	v_{corr}	IE	θ
			[$\mu\text{A cm}^{-2}$]	[mV]	[mV dec $^{-1}$]	[mV dec $^{-1}$]	[mm y $^{-1}$]	[%]	
Al	298	BS	32.9 $\pm$ 0.60	−556 $\pm$ 3.83	534.9 $\pm$ 6.10	649 $\pm$ 5.30	0.358 $\pm$ 0.007	0.0	0.00
		10 $^{-6}$ M	19.9 $\pm$ 0.44	−549 $\pm$ 2.90	328.5 $\pm$ 5.30	364.8 $\pm$ 3.50	0.217 $\pm$ 0.005	39.3	0.39
		10 $^{-5}$ M	13.5 $\pm$ 0.66	−546 $\pm$ 1.53	173.2 $\pm$ 1.20	292.5 $\pm$ 6.30	0.146 $\pm$ 0.008	59.0	0.59
		10 $^{-4}$ M	6.2 $\pm$ 0.21	−526 $\pm$ 1.29	169.5 $\pm$ 2.80	205.7 $\pm$ 5.50	0.067 $\pm$ 0.002	81.2	0.81
		2.5 · 10 $^{-4}$ M	4.3 $\pm$ 0.51	−493 $\pm$ 1.20	123.8 $\pm$ 4.20	127.1 $\pm$ 1.30	0.047 $\pm$ 0.005	86.9	0.87
		5 · 10 $^{-4}$ M	2.8 $\pm$ 0.17	−410 $\pm$ 0.88	47 $\pm$ 1.10	52.3 $\pm$ 2.70	0.03 $\pm$ 0.002	91.5	0.91
	308	BS	33.7 $\pm$ 3.06	−561 $\pm$ 3.02	554 $\pm$ 3.00	704 $\pm$ 17.3	0.367 $\pm$ 0.033	0.0	0.00
		10 $^{-6}$ M	21.9 $\pm$ 0.48	−550 $\pm$ 3.54	337 $\pm$ 1.90	392 $\pm$ 5.50	0.238 $\pm$ 0.005	35.0	0.35
		10 $^{-5}$ M	13.5 $\pm$ 0.95	−551 $\pm$ 3.39	503 $\pm$ 4.10	404.2 $\pm$ 10.5	0.147 $\pm$ 0.010	59.9	0.60
		10 $^{-4}$ M	7.6 $\pm$ 0.04	−510 $\pm$ 2.00	276 $\pm$ 0.80	238 $\pm$ 3.40	0.082 $\pm$ 0.001	77.6	0.78
		2.5 · 10 $^{-4}$ M	5.4 $\pm$ 0.41	−509 $\pm$ 2.25	145 $\pm$ 1.00	129 $\pm$ 1.80	0.059 $\pm$ 0.005	83.9	0.84
		5 · 10 $^{-4}$ M	3.0 $\pm$ 0.03	−447 $\pm$ 1.79	72.7 $\pm$ 6.90	68.2 $\pm$ 3.10	0.033 $\pm$ 0.001	91.0	0.91
	318	BS	33.8 $\pm$ 0.73	−567 $\pm$ 3.51	598 $\pm$ 2.90	641 $\pm$ 3.00	0.368 $\pm$ 0.008	0.0	0.00
		10 $^{-6}$ M	24.5 $\pm$ 0.11	−546 $\pm$ 1.00	379 $\pm$ 6.30	452 $\pm$ 2.80	0.267 $\pm$ 0.001	27.5	0.28
		10 $^{-5}$ M	17.0 $\pm$ 0.12	−546 $\pm$ 1.84	269.8 $\pm$ 2.10	311 $\pm$ 4.70	0.225 $\pm$ 0.024	49.7	0.50
		10 $^{-4}$ M	9.8 $\pm$ 0.72	−522 $\pm$ 1.39	116.7 $\pm$ 1.76	94.5 $\pm$ 0.30	0.106 $\pm$ 0.008	71.1	0.71
		2.5 · 10 $^{-4}$ M	6.5 $\pm$ 0.27	−501 $\pm$ 1.25	74 $\pm$ 3.70	93 $\pm$ 4.50	0.071 $\pm$ 0.003	80.7	0.81
		5 · 10 $^{-4}$ M	5.0 $\pm$ 0.13	−488 $\pm$ 2.00	73.5 $\pm$ 2.40	68.4 $\pm$ 2.00	0.054 $\pm$ 0.002	85.2	0.85
	328	BS	34.4 $\pm$ 0.95	−570 $\pm$ 2.89	557 $\pm$ 9.00	718 $\pm$ 2.10	0.375 $\pm$ 0.010	0.0	0.00
		10 $^{-6}$ M	25.4 $\pm$ 0.46	−517 $\pm$ 1.13	383.1 $\pm$ 5.30	501.5 $\pm$ 2.7	0.277 $\pm$ 0.005	26.1	0.26
		10 $^{-5}$ M	17.1 $\pm$ 0.91	−552 $\pm$ 2.91	337 $\pm$ 2.40	280 $\pm$ 5.20	0.186 $\pm$ 0.010	50.4	0.50
		10 $^{-4}$ M	11.0 $\pm$ 0.40	−524 $\pm$ 0.46	126 $\pm$ 6.00	179 $\pm$ 4.60	0.12 $\pm$ 0.005	68.0	0.68
		2.5 · 10 $^{-4}$ M	7.5 $\pm$ 0.69	−515 $\pm$ 2.22	126 $\pm$ 2.40	176 $\pm$ 1.10	0.081 $\pm$ 0.008	78.2	0.78
		5 · 10 $^{-4}$ M	5.7 $\pm$ 0.04	−491 $\pm$ 1.65	93.3 $\pm$ 1.20	97.3 $\pm$ 0.40	0.062 $\pm$ 0.001	83.4	0.83

3.3. Arrhenius and Eyring Plots

To determine the activation energy (E_a), enthalpy (ΔH_a), and activation entropy (ΔS_a), the slopes derived from the Arrhenius and Eyring representations ($\log i_{corr}$ and $\log(i_{corr}/T)$) as a function of $1000/T$ were utilized. The relationship between corrosion current density and temperature is shown by Equation (7) [33].

$$i_{corr} = Ae^{-E_a/RT} \quad (7)$$

where

i_{corr} —corrosion current density [A m^{-2}], A —preexponential factor, E_a —apparent activation energy [J mol^{-1}], R —universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), T —absolute temperature [K].

To better understand the corrosion process, we applied the logarithm of the Eyring transition-state theory expression (Equation (8)), which delineates the electrochemical reaction rate [34]:

$$\log\left(\frac{i_{corr}}{T}\right) = \log\left(\frac{R}{Nh}\right) + \frac{\Delta S_a}{2.303R} - \frac{\Delta H_a}{2.303RT} \quad (8)$$

where

N —Avogadro number ($6.022 \times 10^{23} \text{ mol}^{-1}$), h —Planck constant ($6.626 \times 10^{-34} \text{ J}\cdot\text{s}$), ΔH_a —apparent activation enthalpy (J mol^{-1}), ΔS_a —apparent activation entropy ($\text{J mol}^{-1} \text{ K}^{-1}$).

The apparent entropy of activation may be determined from the slope of the graphic representation of the $\log(i_{corr}/T)$ function shown versus $1000/T$ [33,34]. The Arrhenius and Eyring diagrams for OLC52 and Al (Figures 8 and 9) were represented using current densities obtained from linear voltammetry within a temperature range of 298 to 328 K, both in the absence and presence of $5 \cdot 10^{-4} \text{ mol L}^{-1}$ YHB.

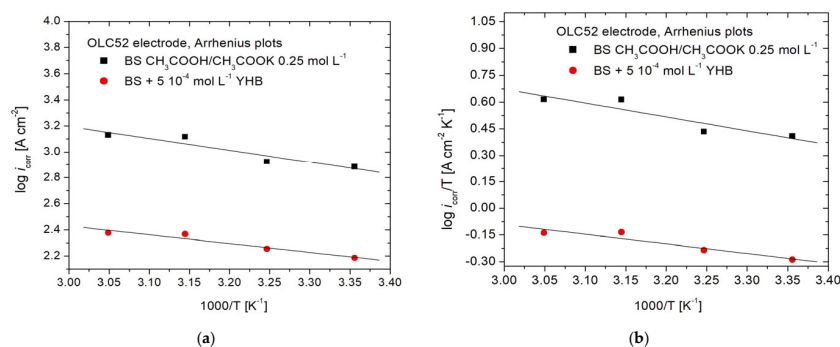


Figure 8. Arrhenius and transition-state plots for OLC52 carbon steel in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ $0.25/0.25 \text{ mol} \cdot \text{L}^{-1}$ solutions, in the absence and presence of $5 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$ YHB: (a) $\log i_{\text{corr}}$ vs. $1000/T$ (Arrhenius plot) and (b) $\log (i_{\text{corr}}/T)$ vs. $1000/T$ (transition-state plot).

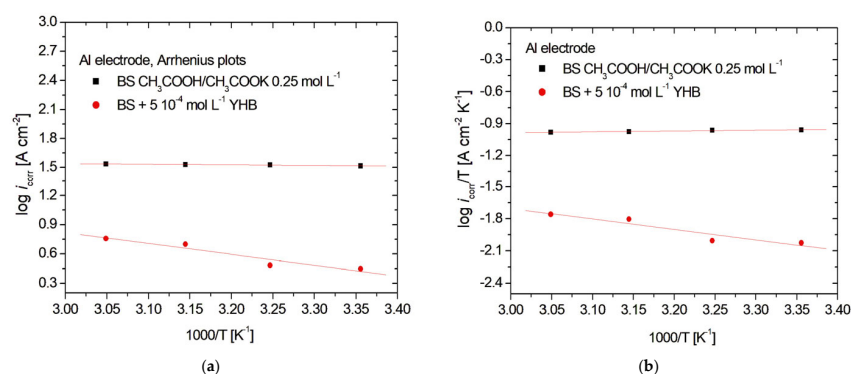


Figure 9. Arrhenius and transition-state plots for Al in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ $0.25/0.25 \text{ mol} \cdot \text{L}^{-1}$ solutions, in the absence and presence of $5 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$ YHB: (a) $\log i_{\text{corr}}$ vs. $1000/T$ (Arrhenius plot) and (b) $\log (i_{\text{corr}}/T)$ vs. $1000/T$ (transition-state plot).

For OLC52, the data in Table 4 indicates that the values of apparent activation energy are appropriate, which indicates that the corrosion mechanism remains unchanged. The presence of the YHB inhibitor slightly slows down the process, attributable to the adsorption of the inhibitor. The marginal reduction in ΔH_a and the increase in the ΔS_a value suggest an enhancement in order at the interface, signifying the development of a thermodynamically favorable compact adsorptive layer with an oriented distribution of YHB molecules.

Table 4. Thermodynamic activation parameters for OLC52 corrosion in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ $0.25/0.25 \text{ mol} \cdot \text{L}^{-1}$.

Electrode	Solution	E_a [kJ mol ⁻¹]	ΔH_a [kJ mol ⁻¹]	ΔS_a [J mol ⁻¹ K ⁻¹]
OLC52	BS (blank)	17.50	14.906	-139.97
	BS + $5 \cdot 10^{-4} \text{ mol L}^{-1}$ YHB	16.99	14.394	-166.31

The results presented in Table 5 concerning aluminum corrosion indicate an increase in activation energy from 1.16 to $21.30 \text{ kJ mol}^{-1}$, underscoring an increased energy barrier for the dissolution process attributed to enhanced passivation and the development of an organic oxide inhibitory layer. The negative apparent activation enthalpy $\Delta H_a = -1.44 \text{ kJ mol}^{-1}$, in the absence of the inhibitor, signifies that the corrosion process of aluminum in the working corrosion media is marginally exoergic, releasing a minor quantity of energy as Al^{3+} ions enter the solution. In contrast, the presence of YHB results in a positive apparent activation enthalpy assumes a positive value (18.7 kJ mol^{-1}), indicating the establishment of a persistent inhibitory layer that diminishes the accessibility of corrosive ions to the metal surface. The rise in order at the interface, indicated by the ΔS_a

value, signifies the systematic spatial arrangement of the adsorbed YHB molecules. These activation parameters also provide useful information about the adsorption mechanism. The positive values of ΔH_a and the increase in E_a in the presence of YHB show an endoenergetic process associated with the formation of a protective layer. The negative values of ΔS_a reflect an orderly arrangement of inhibitor molecules at the interface, consistent with a mixed mechanism of physical and chemical adsorption, according to the thermodynamic models reported for organic inhibitors.

Table 5. Thermodynamic activation parameters for Al corrosion in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 $\text{mol}\cdot\text{L}^{-1}$.

Electrode	Solution	E_a [kJ mol^{-1}]	ΔH_a [kJ mol^{-1}]	ΔS_a [J $\text{mol}^{-1}\text{K}^{-1}$]
Al	BS (blank)	1.16	−1.44	−220.71
	BS + $5 \cdot 10^{-4}$ mol L^{-1} YHB	21.30	18.70	−174.10

3.4. Adsorption Isotherms

To assess the nature and intensity of the interactions between YHB molecules and the investigated metal surfaces, various adsorption models were examined—Langmuir, Freundlich, Temkin, Frumkin, Flory–Huggins, El-Awady, Dubinin–Radushkevich, Volmer, and Hill de Boer—utilizing experimental i_{corr} data obtained from linear voltammetry studies, at the range of concentrations used in electrochemical tests ($10^{-6} \div 5 \cdot 10^{-4}$ M) [35]. The isotherms mentioned are based on different types of assumptions from a physical–chemical point of view. The Freundlich equation describes adsorption on sites that are not equivalent. The Temkin and Frumkin isotherms take into account that the adsorption takes place on the most favorable places on the metal surface, namely the adsorbate–adsorbate and adsorbate–surface interactions. The Flory–Huggins addresses the number of water molecules substituted by an inhibitor molecule. The El-Awady model discusses the potential for the formation of a multimolecular layer at the metal/electrolyte interface. The Dubinin–Radushkevich pertains to adsorption on heterogeneous surfaces, characterized by a Gaussian distribution of site energies, typically correlated with a physical adsorption mechanism. In contrast, the Volmer and Hill-De-Boer models address single-layer adsorption at low surface coverage, with the latter incorporating lateral interactions among the adsorbed molecules [35].

Upon analyzing the correlation values (R^2) of the linear models, as the goodness of fit criteria, it was determined that the Langmuir isotherm (Figure 10a,b) most accurately represents the adsorption of YHB on carbon steel OLC52 and aluminum in an acetic/acetate medium at temperatures ranging from 298 to 328 K.

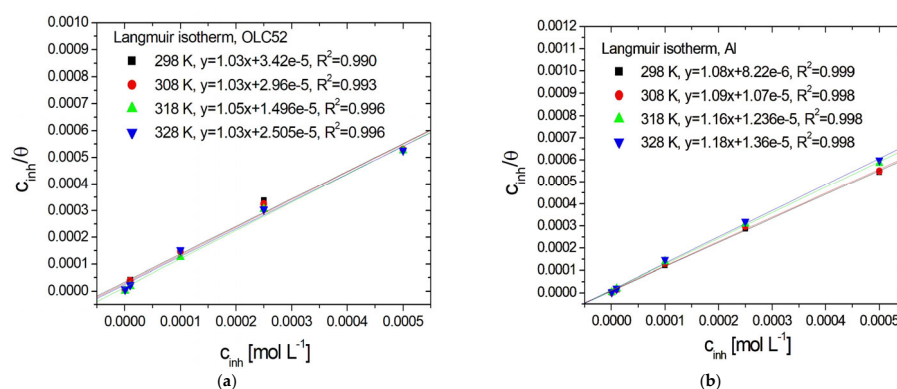


Figure 10. Langmuir adsorption isotherms for YHB on (a) OLC52 and (b) Al in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 $\text{mol}\cdot\text{L}^{-1}$ at 298–328 K.

The surface coverage θ was determined from the corrosion current densities obtained by the Tafel slope method using Equation (9):

$$\theta = \frac{i_{corr,BS} - i_{corr,inh}}{i_{corr,BS}} \quad (9)$$

where $i_{corr,BS}$ and $i_{corr,inh}$ are the corrosion current densities in the absence, respectively, in the presence of YHB. The θ values were subsequently used for the construction of the linear representations of the isotherms.

The Langmuir model asserts the formation of a perfect adsorption monolayer, characterized by minimal lateral interactions between inhibitor molecules, as illustrated by the linearized form (Equation (10)) [35]:

$$\frac{c_{inh}}{\theta} = \frac{1}{K_{ads}} + c_{inh} \quad (10)$$

where c_{inh} represents the concentration of the inhibitor (mol L^{-1}), θ —the degree of coverage of the metal surface, K_{ads} —adsorption equilibrium constant [35].

The graphical representations in Figure 10 indicate a significant correlation between the experimental and theoretical values ($R^2 = 0.99\text{--}0.996$), and the slope values are appropriate for the unit, affirming the validity of the Langmuir model for the examined scenarios. The adsorption constants K_{ads} were ascertained from the y-intercepts of the lines ($1/K_{ads}$), and the standard free energy of adsorption was determined using Equation (11) [35,36].

$$\Delta G_{ads}^0 = -RT \ln(55.55 K_{ads}) \quad (11)$$

where R —universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), and T —absolute temperature (K).

The results of isotherms fitting and the values of ΔG_{ads}^0 for the two metals studied are presented in Table 6.

Table 6. Values of the adsorption equilibrium constant (K_{ads}), standard free energy of adsorption (ΔG_{ads}^0), and correlation coefficient (R^2) for the adsorption of the inhibitor on OLC52 and Al electrodes at different temperatures.

Electrode	T [K]	K_{ads}	ΔG_{ads}^0 [kJ mol ^{−1}]	R^2	RMS Residual c_{inh}/θ
OLC52	298	$2.92 \cdot 10^4$	−35.43	0.990	$2.72 \cdot 10^{-5}$
	308	$3.38 \cdot 10^4$	−36.99	0.993	$2.25 \cdot 10^{-5}$
	318	$6.68 \cdot 10^4$	−39.99	0.996	$1.59 \cdot 10^{-5}$
	328	$3.99 \cdot 10^4$	−39.85	0.996	$1.84 \cdot 10^{-5}$
Al	298	$1.22 \cdot 10^5$	−38.96	0.999	$6.12 \cdot 10^{-6}$
	308	$9.35 \cdot 10^4$	−39.60	0.998	$9.20 \cdot 10^{-6}$
	318	$8.09 \cdot 10^4$	−40.50	0.998	$8.09 \cdot 10^{-6}$
	328	$7.35 \cdot 10^4$	−41.51	0.998	$1.03 \cdot 10^{-5}$

RMS residual—root mean square of the Langmuir isotherm fit residuals.

The analysis of the data in Table 6 reveals that the K_{ads} constants indicate spontaneous and stable adsorption. Additionally, the standard free energy of adsorption (ΔG_{ads}^0) values, ranging from −35 to −41 kJ mol^{−1}, suggest that the inhibitor's adsorption at the metal interface is mixed (physicochemical) with a tendency for chemisorption. Although the distinction related to physisorption and chemisorption is based on the interval between −20 to −40 kJ (ΔG_{ads}^0 is an empirical one [37], this criterion remains widely accepted in the recent literature [38,39].

In comparison to the other metals, the K_{ads} values for aluminum are 3–4 times more than those for OLC52, indicating more robust interactions between YHB and aluminum

oxides. The values of $\Delta G^{\circ}_{\text{ads}}$ for both metals grow increasingly negative with rising temperature, indicating enhanced thermal stability of the organic inhibitor layer. In addition, the RMS values of the residues for the fits corresponding to the Langmuir isotherms are very low, usually of the order of 10^{-5} and are randomly distributed around 0 for all working temperatures, in the case of both metals studied, which confirms the absence of significant deviations from linearity and supports the application of the Langmuir model for the studied systems.

3.5. Chronoamperometry Studies

Chronoamperometry is a technique that entails measuring the variation in current density over time at a fixed potential value. This outlines the development and stability of the inhibitory layer at the electrode interface. Chronoamperometric tests were conducted on OLC52 and Al working electrodes in a $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 mol L⁻¹ supporting electrolyte solution, including varying concentrations of YHB. Prior to conducting the chronoamperometric measurements, it was necessary to observe the open circuit potential (OCP) for 3600 s to stabilize the system.

For OLC52 (Figure 11), increased YHB concentrations result in chronoamperometric responses characterized by diminished and more stable currents. At 25 mV from E_{OCP} , the curves exhibit an initial increase, followed by stabilization, which indicates the gradual formation of an adsorbed layer of YHB. At 250 mV versus E_{OCP} , the current decreases from about 50 A m⁻² in BS to about 30 A m⁻² in the presence of YHB, in conjunction with the existence of a compact protective coating that slows anodic dissolution. In the presence of YHB, the current density diminishes to around 30 A m⁻², indicating a decrease in the corrosion rate due to the formation of a compact protective coating.

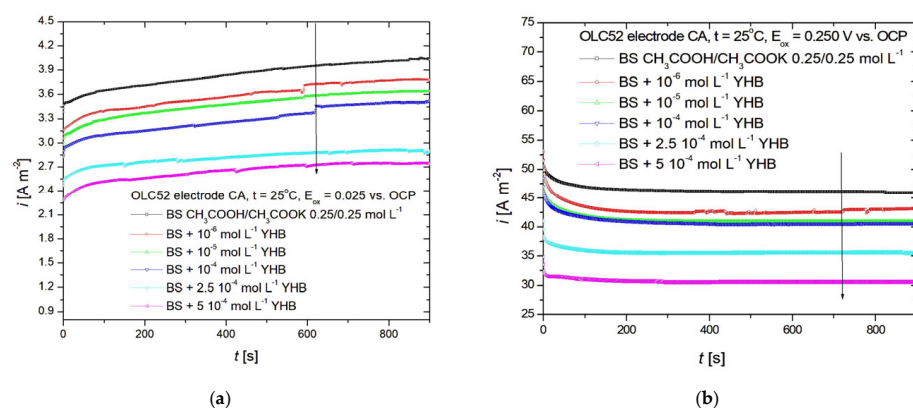


Figure 11. Chronoamperograms recorded on the OLC52 electrode in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ 0.25/0.25 mol·L⁻¹ solution containing different concentrations of YHB at potentials of (a) 25 mV vs. OCP and (b) 250 mV vs. OCP.

In the case of aluminum (Figure 12a,b), we observe a similar increase, albeit with decreasing current density values (1–3 A m⁻²). At 25 mV versus E_{OCP} the current density remains nearly constant (around 0.5 A m⁻²) in the first minutes, which indicates that the aluminum is in an active state of dissolution, not in the formation of a stable passivating oxide layer. At 250 mV versus open circuit potential, in the absence of the inhibitor, a small increase in current is seen due to the dissolution of the Al_2O_3 film. The addition of YHB considerably reduces the current values, indicating the formation of a stable oxide coating that limits charge transfer.

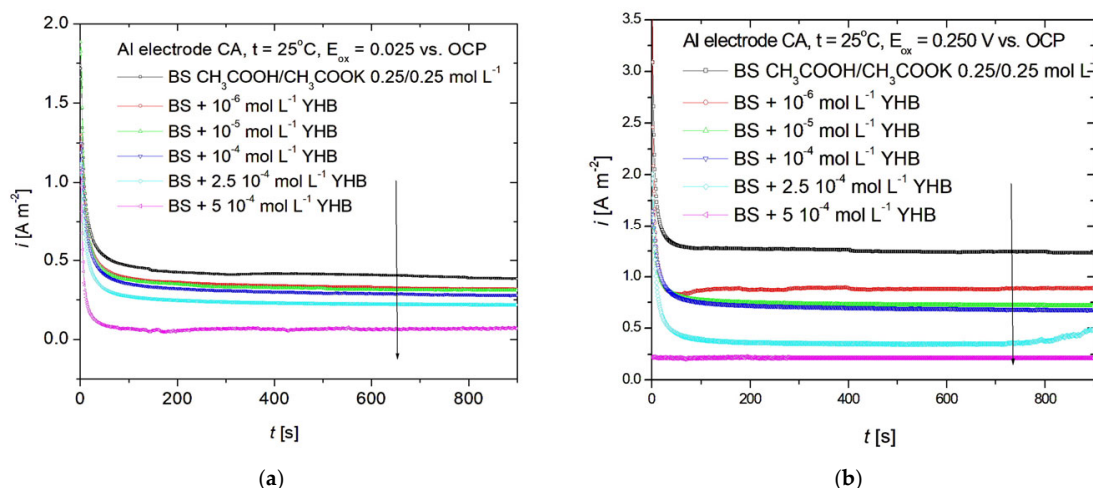


Figure 12. Chronoamperograms recorded on the Al electrode in CH₃COOH/CH₃COOK 0.25/0.25 mol·L⁻¹ solution containing different concentrations of YHB at potentials of (a) 25 mV vs. OCP and (b) 250 mV vs. OCP.

The increasing value of the open circuit potential (Figure 13) in both scenarios confirms that by adjusting the E_{OCP} potential to more positive values, the surface of OLC52 is protected from corrosion, while in the case of aluminum, YHB effectively adsorbs to the aluminum oxide layer, thereby stabilizing the protective film. This behavior aligns with the values obtained from the Langmuir isotherms, indicating a pronounced tendency for adsorption and the establishment of chemical bonds with the metal surface.

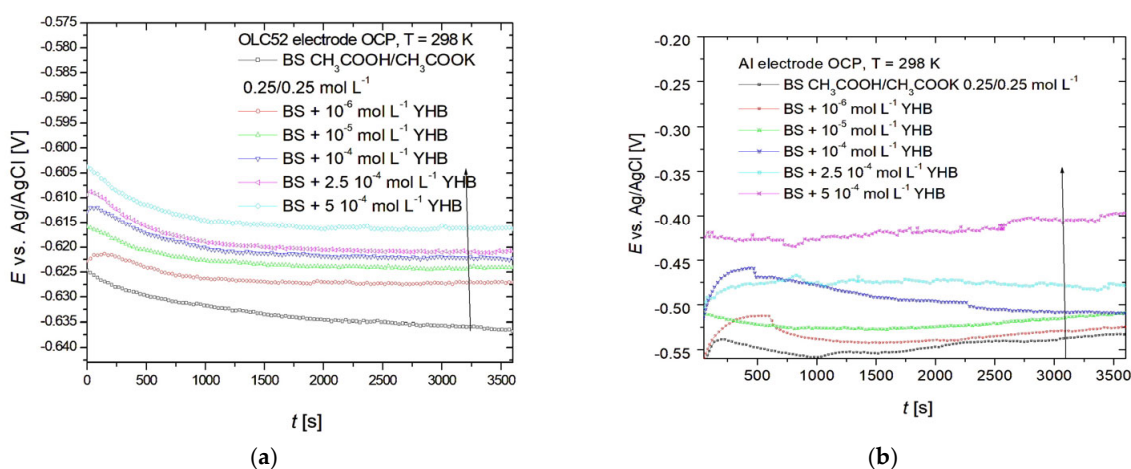


Figure 13. Open circuit potential (OCP) evolution in time for (a) OLC52 and (b) Al electrodes in CH₃COOH/CH₃COOK 0.25/0.25 mol·L⁻¹ solution with and without YHB.

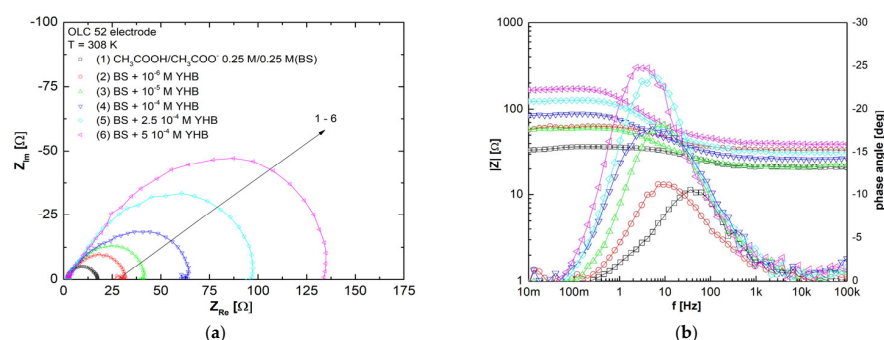
The experimental data in Table 7 indicate that YHB acts as an effective corrosion inhibitor for both metals examined. For OLC52, the data at both working potentials confirm a significant reduction in anodic currents (from 4.2 to 2.4 A m⁻² at 25 mV/ E_{OCP} and from 48 to 32 A m⁻² at 250 mV/ E_{OCP}), as the inhibitor concentration increases, emphasizing the limitation of anodic and cathodic processes through a partial chemical adsorption. For Al, the current at 250 mV/ E_{OCP} decreases from 1.4 to 0.15 A m⁻² at 250 mV/ E_{OCP} and from 0.6 to 0.1 A m⁻² at 25 mV/ E_{OCP} , showing that adsorbed YHB molecules hinder metal dissolution and transiently stabilize the oxide layer.

Table 7. Chronoamperometric and chronopotentiometric data characteristic of carbon steel OLC52 and Al corrosion process in test solutions.

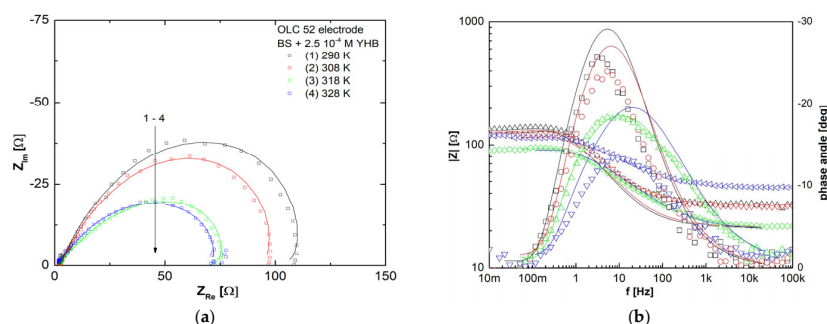
Metal	YHB Concentration	E_{OCP} [mV]/Ref	E_{ox}	
			25 mv/ E_{OCP}	250 mv/ E_{OCP}
			i_{corr} [A m ⁻²]	
OLC52	BS	−635	4.2	48
	10 ^{−6} M	−633	3.8	47
	10 ^{−5} M	−625	3.5	44
	10 ^{−4} M	−621	3.2	42
	2.5 · 10 ^{−4} M	−619	2.9	37
	5 · 10 ^{−4} M	−618	2.4	32
Al	BS	−560	0.6	1.4
	10 ^{−6} M	−535	0.55	0.9
	10 ^{−5} M	−515	0.42	0.8
	10 ^{−4} M	−502	0.4	0.75
	2.5 · 10 ^{−4} M	−482	0.25	0.4
	5 · 10 ^{−4} M	−419	0.1	0.15

3.6. Electrochemical Impedance Spectroscopy Studies

Figure 14a,b present EIS spectra depicted as Nyquist and Bode plots illustrating OLC52 corrosion in CH₃COOH/CH₃COO[−] test solutions in the absence and presence of YHB different concentrations used in experimental studies, at the same temperature value, 35 °C.

**Figure 14.** (a) Nyquist and (b) Bode plots of carbon steel electrode (OLC52) in CH₃COOH/CH₃COO[−] test solutions, in the absence and presence of different concentrations of YHB, at 35 °C (Open symbols show experimental values and continuous lines were obtained by fitting).

Also, in Figure 15a,b are shown EIS spectra (Nyquist and Bode plots) for the case of corrosion studied at same inhibitor concentration (2.5 · 10^{−4} M YHB) added in BS at four temperatures values between 25 °C and 55 °C. The continuous lines were generated by fitting, using a Randles circuit, while open symbols indicate experimental data.

**Figure 15.** (a) Nyquist and (b) Bode plots of carbon steel electrode (OLC 52) in CH₃COOH/CH₃COO[−] test solutions, 2.5 · 10^{−4} M YHB concentration, at different temperature values.

Figures 16 and 17 present the spectra acquired for the measurements conducted on an aluminum electrode at the same working conditions.

The equivalent electrical circuit (EEC) shown in Figure 18 comprises a solution resistance R_s in series with a parallel connection of a constant phase element (CPE), which account for the double layer capacity and a series connection between a charge transfer resistance R_{ct} and magnetic coil (inductor) element. This is a typical electrical circuit for adsorption process of inhibitors on metal surfaces, where chemical species, ions or other molecules are physically adsorbed at the metallic interface of the electrochemical double layer, exhibiting a specific electrical charge motion [40,41].

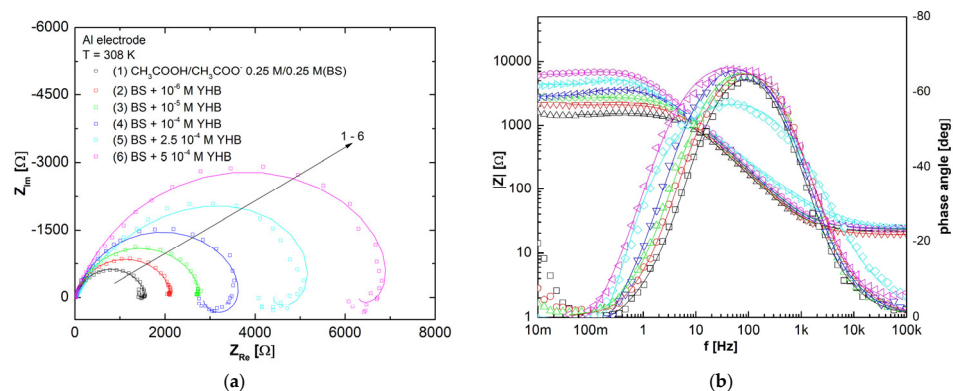


Figure 16. (a) Nyquist and (b) Bode plots of aluminum electrode in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions, in the absence and presence of different concentrations of YHB, at 35°C (open symbols show experimental values and continuous lines were obtained by fitting).

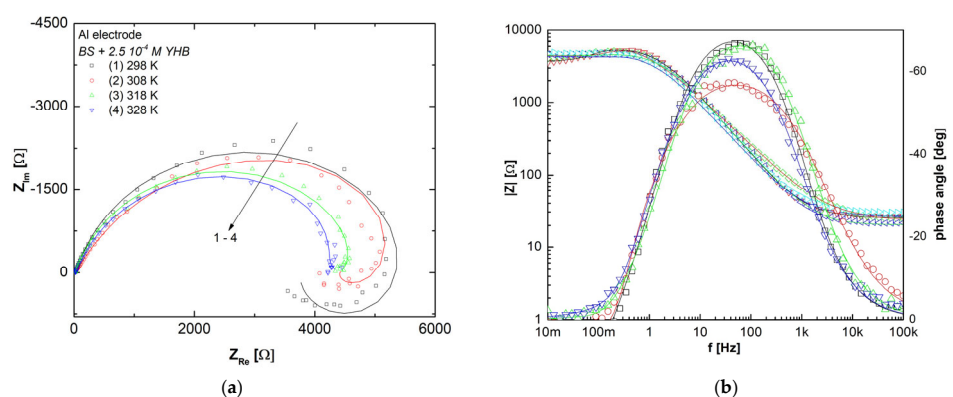


Figure 17. (a) Nyquist and (b) Bode plots of aluminum electrode in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions, $2.5 \cdot 10^{-4}$ M YHB concentration, at different temperature values.

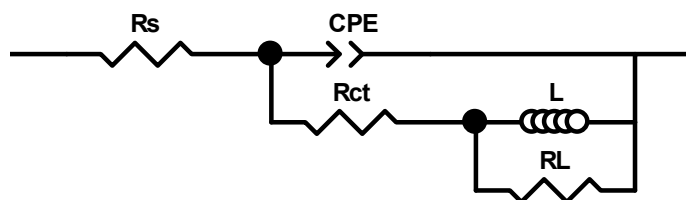


Figure 18. Electrical equivalent circuit (EEC) for modeling OLC 52, an Al corrosion processes, in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions.

The experimental diagrams show a deformed semicircle which describes the charge transfer process followed by a second semicircle at low frequencies which defines the inductance response (more visible in aluminum corrosion case), typical for adsorption

ion mechanism. Inductive loops at low frequencies are frequently attributed to adsorption phenomena at the metal/electrolyte interface; however, recent studies indicate that this kind of behavior can occur from non-steady-state conditions during electrochemical impedance spectroscopy measurements. Wang et al. [42] demonstrated that after attaining a steady open circuit potential, differences exist between the impedance spectra acquired from measurements conducted in opposing frequency directions (from high frequency to low frequency and vice versa). This sort of non-stationarity can provide a pseudo-inductive behavior, particularly in systems where superficial film development occurs. Klotz [43] demonstrated that the inductive signals displayed in the Nyquist spectra originate from charging processes associated with the modification of interfacial resistance; thus, the observed inductive loops may indicate, alongside the effects of inhibitor adsorption, additional intricate interfacial dynamics.

The resistance R_s component represents the uncompensated solution resistance. In the EEC utilized for simulating the OLC52 corrosion process, the ideal capacitor characterized by double layer capacity (C_{dl}) is substituted by a constant phase element (CPE) since it more accurately reflects the behavior of real electrochemical systems, particularly of depressed loops in EIS spectra.

The impedance of the constant phase element is delineated in Equation (12) [42].

$$Z_{CPE} = 1/T(j\omega)^n \quad (12)$$

where T is a parameter proportional to the capacitance of the double layer and n , ranging from 0 to 1, describes the deviation from the ideal capacitive behavior [44,45]. For the OLC52 electrode, the CPE- n exponents obtained by fitting the EIS data (Tables 8 and 9) decrease from 0.73 in BS to 0.61 at the highest YHB concentration and from 0.65 to 0.52 as the temperature increases from 298 to 328 K, in the case of the fixed inhibitor concentration ($2.5 \cdot 10^{-4}$ M). For the Al electrode, n varies between 0.84 and 0.78 in the concentration series shown in Table 10 and between 0.82 and 0.76 in the temperature series. These deviations from the ideal value $n = 1$ quantitatively describe the depression of capacitive semicircles in Nyquist diagrams, indicating an unideal capacitive behavior associated with surface heterogeneity and the formation of adsorbed films. The capacitance of the electrochemical double layer (C_{dl}) was determined using Equation (13) [45].

$$C_{dl} = T^{1/n} \left(\frac{1}{R_s} - \frac{1}{R_{ct}} \right)^{\frac{n-1}{n}} \quad (13)$$

Table 8. Impedance parameters for carbon steel electrode corrosion at 35 °C in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions in the absence and presence of varying concentrations of YHB calculated by fitting the experimental data.

YHB Conc. (M)	R_s (Ω)	CPE- T ($\text{F cm}^{-2} \text{ s}^{n-1}$) $\cdot 10^3$	n	R_{ct} ($\Omega \text{ cm}^2$)	χ^2	L (H cm^2)	R_L ($\Omega \text{ cm}^2$)	$C_{dl} \cdot 10^4$ ($\mu\text{F cm}^{-2}$)	E (%)	θ
BS	1.85 (0.17%)	1.73 (2.51%)	0.73 (1.10%)	19.42 (0.69%)	0.56×10^{-3}	1.07 (2.83)	7.831 (5.13)	2.08	–	–
10^{-6}	1.65 (0.28%)	2.55 (3.78%)	0.66 (1.13%)	29.17 (0.71%)	1.99×10^{-3}	2.38 (1.19)	4.548 (0.89)	1.50	33.4	0.33
10^{-5}	1.90 (0.17%)	2.93 (2.32%)	0.64 (0.74%)	40.49 (0.71%)	0.41×10^{-3}	2.81 (0.83)	7.775 (0.65)	1.63	52.0	0.52
10^{-4}	1.58 (0.35%)	3.00 (2.55%)	0.64 (0.93%)	61.36 (0.69%)	2.03×10^{-3}	20.9 (0.87)	13.22 (0.67)	1.50	68.4	0.68
2.5 $\cdot 10^{-4}$	1.98 (0.43%)	3.12 (3.04%)	0.63 (1.00%)	91.58 (1.00%)	1.91×10^{-3}	16.5 (0.99)	25.29 (0.94)	1.67	78.8	0.79
$5 \cdot 10^{-4}$	2.36 (0.59%)	3.21 (3.22%)	0.61 (1.15%)	169.8 (0.97%)	3.93×10^{-3}	49.2 (0.82)	51.29 (0.95)	1.51	88.6	0.87

Table 9. Impedance parameters for carbon steel electrode corrosion at test temperatures in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ solutions in the absence and presence of varying concentrations of YHB calculated by fitting the experimental data.

T (K)	R_s (Ω)	CPE-T ($\text{F cm}^{-2} \text{ s n}^{-1}$) $\cdot 10^3$	n	R_{ct} ($\Omega \text{ cm}^2$)	χ^2	L (L cm^2)	R_L ($\Omega \text{ cm}^2$)	$C_{dl} \cdot 10^4$ ($\mu\text{F cm}^{-2}$)
298	2.19 (0.55%)	2.05 (3.51%)	0.65 (1.21%)	107.7 (1.16%)	3.88×10^{-3}	26.85 (1.25)	31.05 (1.08)	1.11
308	1.98 (0.43%)	3.12 (3.04%)	0.63 (1.03%)	91.58 (1.00%)	1.91×10^{-3}	16.5 (0.99)	25.29 (0.94)	1.67
318	1.58 (0.56%)	3.25 (3.22%)	0.57 (0.27%)	79.18 (1.11%)	1.13×10^{-3}	18.44 (0.77)	26.79 (0.80)	0.84
328	1.18 (0.51%)	3.42 (3.35%)	0.52 (1.12%)	75.42 (1.32%)	0.87×10^{-3}	7.36 (1.44)	14.26 (0.96)	0.83

Table 10. Impedance parameters for aluminum electrode corrosion at 35 °C in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions in the absence and presence of varying concentrations of YHB calculated by fitting the experimental data.

YHB Conc. (M)	R_s (Ω)	CPE-T ($\text{F cm}^{-2} \text{ s n}^{-1}$) $\cdot 10^5$	n	R_{ct} ($\Omega \text{ cm}^2$)	χ^2	L (L cm^2)	R_L ($\Omega \text{ cm}^2$)	$C_{dl} \cdot 10^6$ ($\mu\text{F cm}^{-2}$)	E (%)	θ
BS	2.79 (0.46%)	2.63 (1.48%)	0.84 (0.26%)	1044 (0.90%)	2.04×10^{-3}	100.7 (2.34)	141 (1.01)	4.47	—	—
10^{-6}	2.05 (0.43%)	2.57 (1.25%)	0.83 (0.22%)	1700 (0.94%)	1.28×10^{-3}	525.6 (3.47)	307 (1.66)	4.03	38.6	0.39
10^{-5}	4.17 (0.54%)	2.53 (1.53%)	0.83 (0.28%)	2518 (0.93%)	2.08×10^{-3}	973.5 (4.78)	638 (2.19)	3.68	58.5	0.59
10^{-4}	4.68 (0.70%)	2.47 (1.74%)	0.82 (0.32%)	3629 (1.01%)	3.48×10^{-3}	1449 (0.49)	1037 (0.41)	3.31	71.2	0.71
$2.5 \cdot 10^{-4}$	4.46 (1.09%)	2.38 (2.00%)	0.79 (0.43%)	4962 (1.09%)	5.27×10^{-3}	1651 (0.68)	1149 (0.64)	3.04	79.0	0.79
$5 \cdot 10^{-4}$	3.36 (0.77%)	2.26 (1.58%)	0.78 (0.31%)	7314 (1.09%)	4.38×10^{-3}	2148 (1.46)	1387 (0.77)	2.72	87.7	0.88

The IE values of YHB compound were determined using the charge transfer resistance (R_{ct}) values from Tables 8 and 9 for OLC 52 and Tables 10 and 11 for aluminum, following Equation (14), where R_{ct}^0 and R_{ct}^i are the charge transfer resistance in BS, respectively, without and with different YHB concentrations.

$$IE (\%) = \frac{\left(\frac{1}{R_{ct}^0}\right) - \left(\frac{1}{R_{ct}^i}\right)}{\left(\frac{1}{R_{ct}^0}\right)} \times 100 \quad (14)$$

Table 11. Impedance parameters for aluminum electrode corrosion at different temperature values in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions with $2.5 \cdot 10^{-4}$ M YHB concentration calculated by fitting the experimental data.

T (K)	R_s (Ω)	CPE-T ($\text{F cm}^{-2} \text{ s n}^{-1}$) $\cdot 10^3$	n	R_{ct} ($\Omega \text{ cm}^2$)	χ^2	L (L cm^2)	R_L ($\Omega \text{ cm}^2$)	$C_{dl} \cdot 10^4$ ($\mu\text{F cm}^{-2}$)
298	6.47 (0.70%)	2.11 (1.60%)	0.82 (0.31%)	5291 (1.12%)	3.34×10^{-3}	3499 (2.04)	2093 (3.11)	4.03
308	4.46 (1.09%)	2.38 (2.00%)	0.79 (0.43%)	4962 (1.09%)	5.27×10^{-3}	1651 (2.81)	1649 (4.38)	3.04
318	1.25 (0.67%)	2.97 (1.55%)	0.78 (0.29%)	4465 (0.83%)	3.41×10^{-3}	470 (2.42)	974 (2.65)	2.47
328	7.39 (0.39%)	3.93 (0.99%)	0.76 (0.20%)	4228 (0.46%)	1.05×10^{-3}	371 (1.02)	669 (2.54)	1.97

The semicircle diameter correlates with the R_{ct} value, which significantly increases with YHB concentration, suggesting that charge transfer is impeded in its presence. The typical frequency of the charge transfer process shifts to lower values as YHB concentration increases, further substantiating this observation. In the intermediate frequency range, the curves $|Z|$ vs. f for OLC52 in Figure 14b exhibit slopes approximately between -0.6 and -0.7 , and the phase angle has a single wide maximum of about 60 – 70° , in accordance with the values of the CPE exponent of 0.73 – 0.61 in Tables 8 and 9. In the case of the Al electrode (Figures 16b and 17b), the slopes in the intermediate frequency range are appropriate from -0.8 to -0.9 , and the phase angle maximums reach about 70 – 80° . The quantitative characteristics of the Bode diagrams confirm the existence of a response time dominated

by charge transfer and the formation of a more capacitive protective surface film in the presence of YHB. In the process illustrated by the EEC in Figure 18, the R_{ct} value is directly proportional to the corrosion resistance of OLC52 samples in $\text{CH}_3\text{COOH}/\text{CH}_3\text{COO}^-$ test solutions [46]. The data from Tables 8 and 10 unequivocally demonstrates that R_{ct} rises with higher concentrations of YHB in test solutions, corroborating the results from linear polarization tests. The chi-square values around 10^{-3} demonstrate a strong correlation between the EIS experimental data and the values derived from the EEC model. It should be underlined that moderate discrepancies between inhibitory efficiencies determined by Tafel/PDP measurements and those obtained by EIS are frequently reported in the literature. In this case, the IE values for Al obtained from R_{ct} (88%) and from i_{corr} corrosion currents of the Tafel slope method fall within this typical experimental scatter, which indicates that the results of the EIS and Tafel are consistent and mutually reinforcing.

3.7. Molecular Modeling

Theoretical molecular modeling calculations were conducted to comprehend the behavior of YHB molecules at the metal/aggressive solution interface and to correlate the electronic structure with the experimentally determined IE. Figure 19 illustrates the optimal configuration of the YHB molecules used in the experimental tests. The arrow, marked with the orientation from negative to positive, signifies the direction of the dipole moment, while the atoms are depicted as follows: red for oxygen, cyan for carbon, blue for nitrogen, and white for hydrogen.

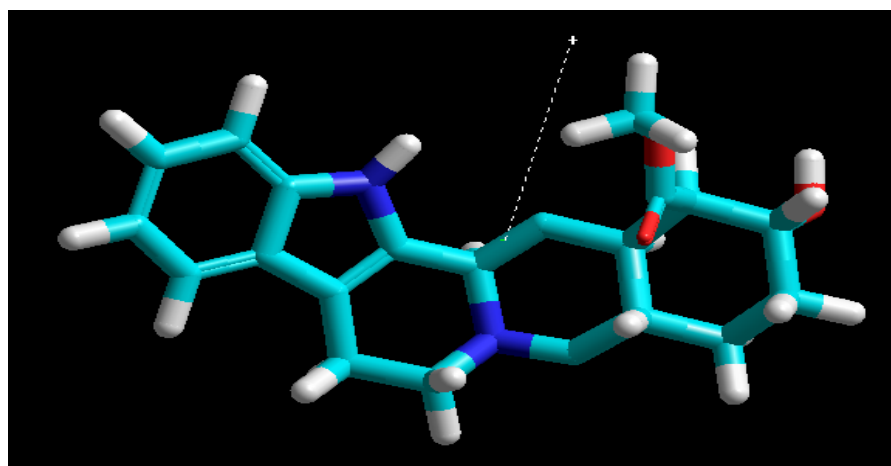


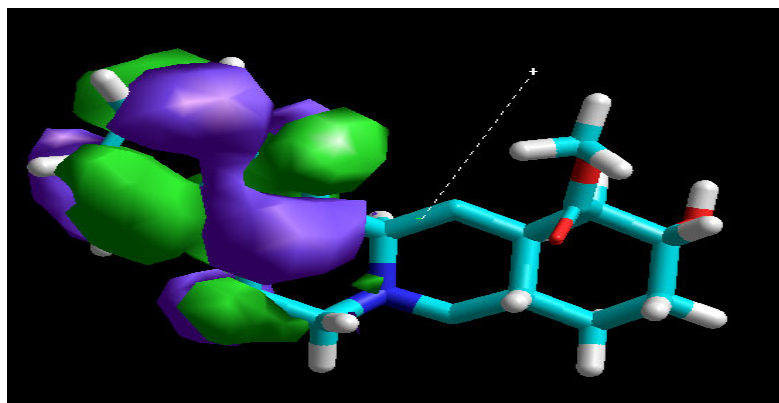
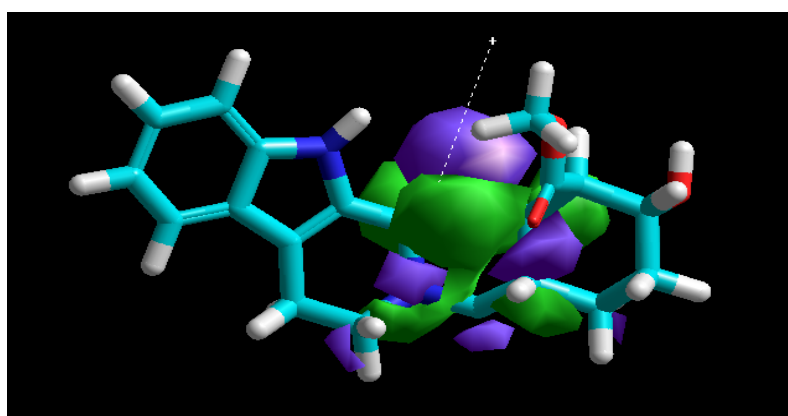
Figure 19. Optimized structure of the YHB molecule.

For quantum calculations, the Density Functional Theory—DFT—was used, implemented in the Hyperchem 8.0 software, utilizing the B3LYP function with the 6-31G* base set. The geometry optimization was performed for the neutral molecule of YHB in its ground state—total charge = 0, spin multiplicity = 1, closed-shell singlet, using the default convergence criteria from Hyperchem, namely the following: the SCF procedure was iterated until the total energy variation between successive cycles became less than 10^{-6} u.a and the optimization was continued until the mean square gradient decreased below $0.01 \text{ kcal mol}^{-1} \text{ \AA}^{-1}$. The descriptors of the investigated molecule are presented in Table 12. These include the energies of the Frontier orbitals, E_{HOMO} , E_{LUMO} , energy difference ΔE , dipole moment μ , electronegativity χ , chemical hardness η , chemical softness σ , molecular volume V , and surface area of molecule S [47].

Table 12. Molecular descriptors and their values for the YHB molecule.

Molecular Descriptor	Value
E_{HOMO} (eV)	−8.38
E_{LUMO} (eV)	−0.60
ΔE (eV)	7.78
μ (Debye)	2.84
χ (eV)	3.89
η (eV)	4.49
σ (eV ^{−1})	0.22
V [Å ³]	994.73
S [Å ²]	581.72
V/S [Å]	1.71

Figures 20 and 21 show the distribution of the HOMOs and LUMOs. The HOMO is located mostly on the rings that present aromaticity, respectively, nitrogen atoms, illustrating areas with significant electron-donating potential, while the LUMO is aligned with the hydroxy and carbonyl groups, where electron acceptance occurs [48].

**Figure 20.** The structure of the highest energy occupied molecular orbital (HOMO).**Figure 21.** The structure of the lowest energy unoccupied molecular orbital (LUMO).

The E_{HOMO} value of −8.38 eV indicates a substantial stability of YHB and a moderate ability to interact with the metal surface by electron donation, whereas the E_{LUMO} value of −0.60 eV suggests the potential to accept electrons from the vacant orbitals of the analyzed metals. The energy difference $\Delta E = 7.78$ eV corroborates the modest reactivity and stability of the adsorbed layer [49]. The dipole moment value $\mu = 2.84$ D signifies adequate polarity for electrostatic and covalent interactions, while the values $\chi = 3.89$ eV, $\eta = 4.49$ eV, and $\sigma = 0.22$ eV^{−1} underscore a moderately “soft” molecule, elucidating the mixed physico-chemical adsorption observed experimentally [50]. The geometric parameters of the YHB

molecule indicate a volume of $V = 994.73 \text{ \AA}^3$ and a surface area of $S = 581.72 \text{ \AA}^2$, suggesting effective metal surface coating. The V/S ratio of $1.71 \text{ \AA}$ further implies the formation of a compact film that efficiently inhibits corrosion on the examined samples [51].

3.8. Surface Morphology

To correlate the electrochemical results with the morphological changes at the metal surface, 3D optical microscopy investigations were conducted on the OLC52 and Al samples after a 240 h immersion in the test solutions. The examinations were conducted with the Olympus LEXT OLS 4000 confocal microscope at a $50\times$ magnification. Image analysis was conducted with IDS uEye Cockpit software, version 4.20 (IDS Imaging Development Systems GmbH, Obersulm, Germany).

The working samples were immersed in the (BS) and in solutions with YHB concentrations of 10^{-6} , 10^{-5} , and $10^{-4} \text{ mol L}^{-1}$. Figures 22 and 23 depict images acquired from the Al and OLC samples, respectively, after 240 h of exposure. The exposed sample surface without the inhibitor, as shown in Figure 22a, displays a rough and irregular shape characterized by significant flaws indicative of localized corrosion and anodic dissolution processes. With the decreased concentration of the inhibitor, as seen in Figure 22b, a noticeable decrease in roughness is evident due to the initiation of YHB molecule adsorption. At moderate and high concentrations, a gradual uniformity of the surface is evident due to the development of a persistent protective coating that diminishes electrochemical activity. The pattern seen for Al parallels that of OLC52 steel (Figure 23), exhibiting a steady decrease in roughness and attack zones with rising inhibitor concentration. The morphological examination verifies the enhanced efficacy of the YHB inhibitor, demonstrating a notable decrease in roughness corresponding to the inhibitor concentration, hence corroborating the electrochemical investigations.

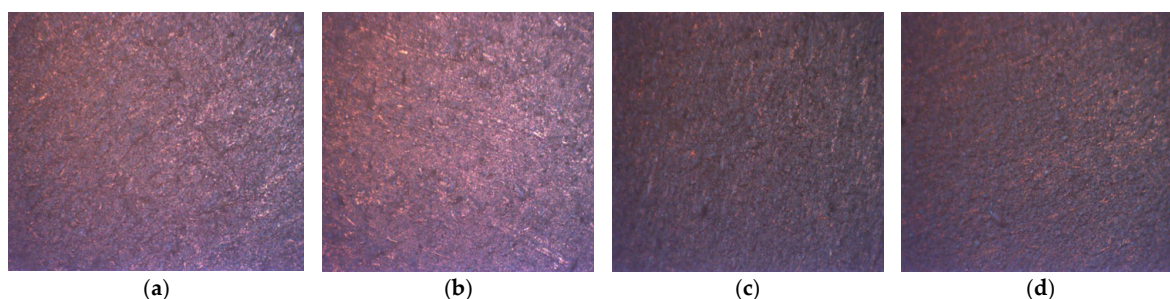


Figure 22. Optical microscopy images of the aluminum surface ($50\times$ magnification) after 240 h of immersion in the following: (a) the base solution $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ $0.25/0.25 \text{ mol L}^{-1}$; (b) BS + 10^{-6} YHB; (c) BS + 10^{-5} YHB; (d) BS + 10^{-4} YHB.

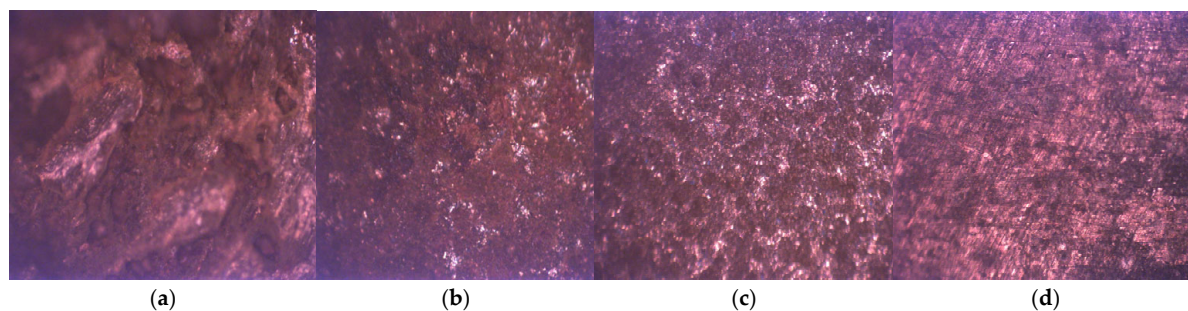


Figure 23. Optical microscopy images of the OLC52 surface ($50\times$ magnification) after 240 h of immersion in the following: (a) the base solution $\text{CH}_3\text{COOH}/\text{CH}_3\text{COOK}$ $0.25/0.25 \text{ mol L}^{-1}$; (b) BS + 10^{-6} YHB; (c) BS + 10^{-5} YHB; (d) BS + 10^{-4} YHB.

4. Conclusions

This study performed the evaluation of the inhibitory efficacy of YHB on the corrosion process of carbon steel type OLC52 and Al in an electrolyte support solution of acetic acid/acetate of concentration 0.25/0.25 mol L⁻¹, using an electrochemical, thermodynamic, and theoretical approach. The results obtained from the study showed that YHB acts as an effective ecological corrosion inhibitor for both materials studied.

From the electrochemical investigations of cyclic voltammetry it was highlighted that YHB manifests electrochemical stability in the potential frame between the hydrogen and oxygen release potentials. Linear voltammetry and chronoamperometry show a systematic decrease in i_{corr} and a shift in the E_{corr} to more positive values, as the YHB concentration increases. The corrosion rate decreased significantly in both metals studied, reaching an IE of 95% for OLC52 and 91% for Al at 298 K.

From the thermodynamic analysis, it was highlighted that the activation energy decreased slightly for OLC52 (from 17.5 to 16.99 kJ mol⁻¹) and increased for Al (from 1.16 to 21.3 kJ mol⁻¹), suggesting the formation of a passivating layer of oxidic nature. From the positive values of enthalpy ΔH_a and negative values of entropy, an endothermic adsorption process is suggested, which involves the formation of an orderly layer of adsorbed molecules.

The modeling of the adsorption isotherms demonstrated that the Langmuir model shows the best fit based on R^2 greater than 0.99 for both cases studied, indicating a monolayer adsorption, and the $\Delta G^\circ_{\text{ads}}$ values between -35 and -41 kJ mol⁻¹ confirm the hypothesis of a spontaneous, predominantly chemical process, due to donor-acceptor interactions between the N and O heteroatoms of the YHB molecule and the vacant orbitals of the metal.

The EIS spectra confirmed that an equivalent circuit (R_s -CPE- R_{ct} -L) adequately describes both systems studied. The increase in YHB concentration led to a higher R_{ct} charge transfer resistance and a decrease in C_{dl} double layer capacitance, which confirms the progressive formation of a protective film on the metal surface.

Quantum molecular modeling calculations have shown that YHB has $E_{\text{HOMO}} = -8.38$ eV and $E_{\text{LUMO}} = -0.60$ eV and a gap $\Delta E = 7.78$ eV. The dipole moment of 2.84 D and the presence of nitrogen functional groups suggest the mixed mechanism of physical and chemical adsorption.

The morphological analysis of the metallic surfaces revealed significant differences between the samples in the electrolyte support solution and those protected by YHB. Microscopic images showed that in the absence of the inhibitor, the surfaces show pronounced corrosion, characterized by pores and localized attack zones. In the presence of YHB, these defects are considerably reduced, the surface being covered by an adherent protective film in accordance with the results from electrochemical and thermodynamic analyses.

In conclusion, YHB exhibits an effective inhibitory behavior, by reducing the corrosion rate by more than 90% under moderate conditions, providing an environmentally friendly alternative for the protection of iron and aluminum alloys in slightly acidic environments.

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Conflicts of Interest: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

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